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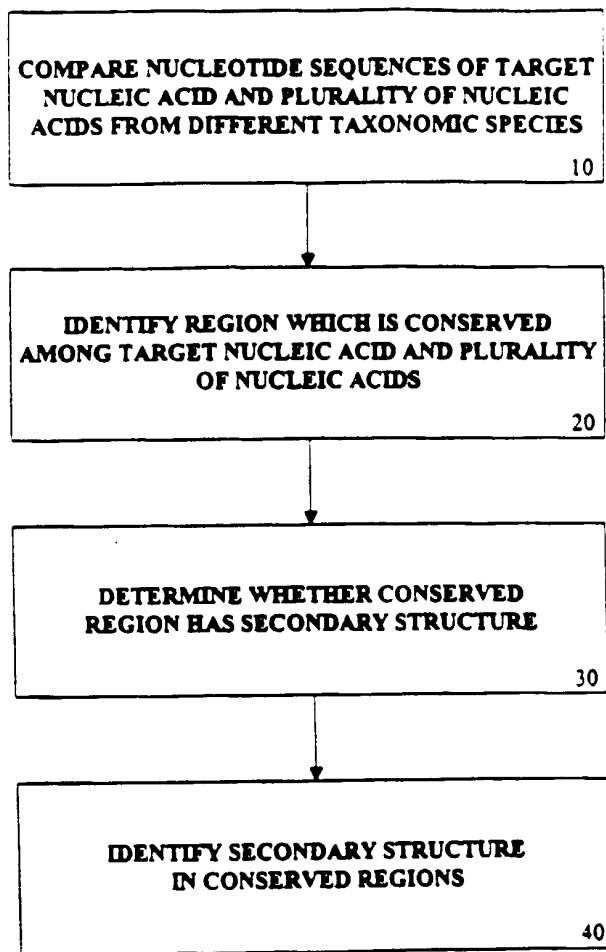


FIGURE 1

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Find Neighbors
and Assemble
Flow Diagram

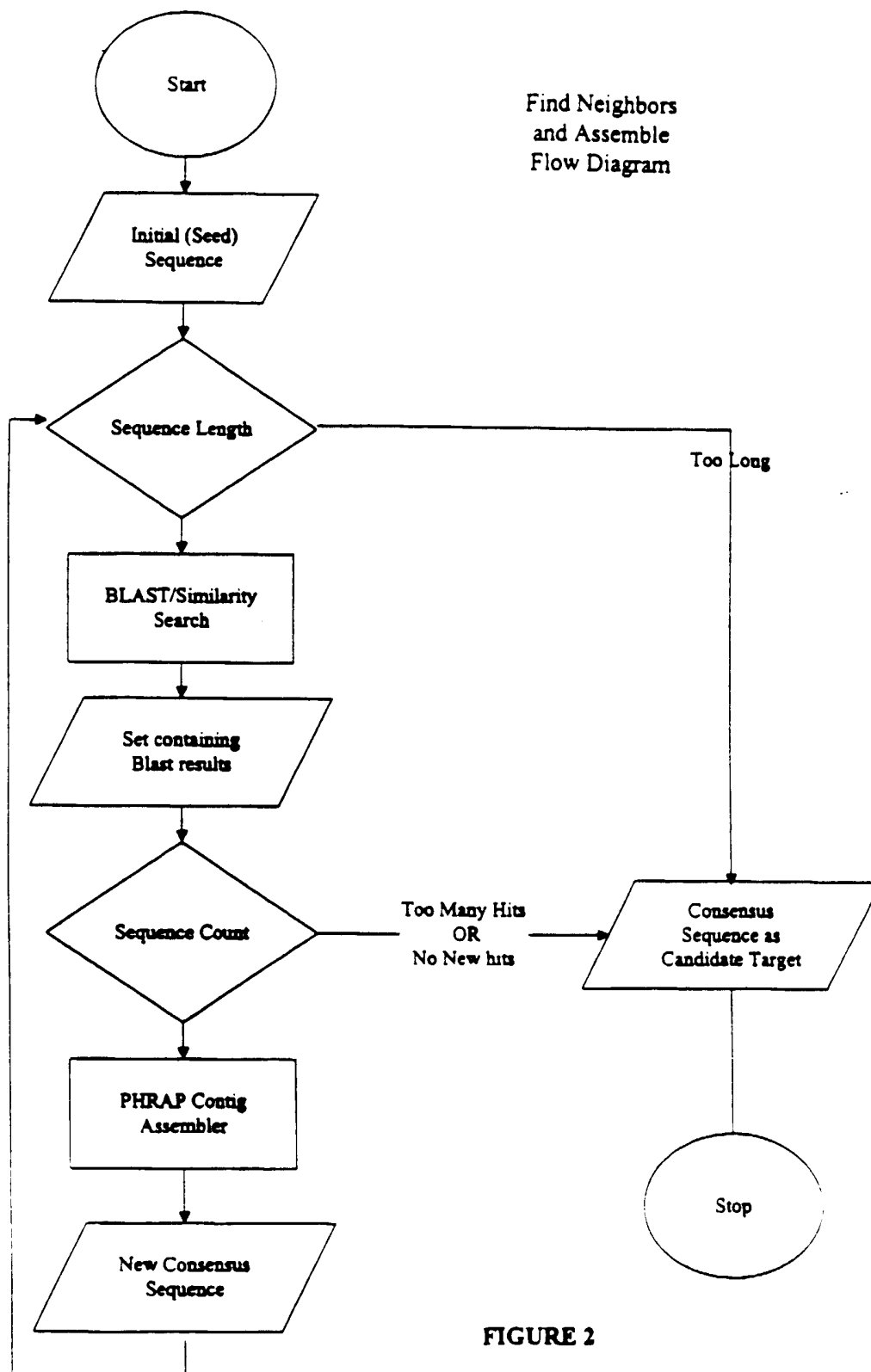


FIGURE 2



Figure 3

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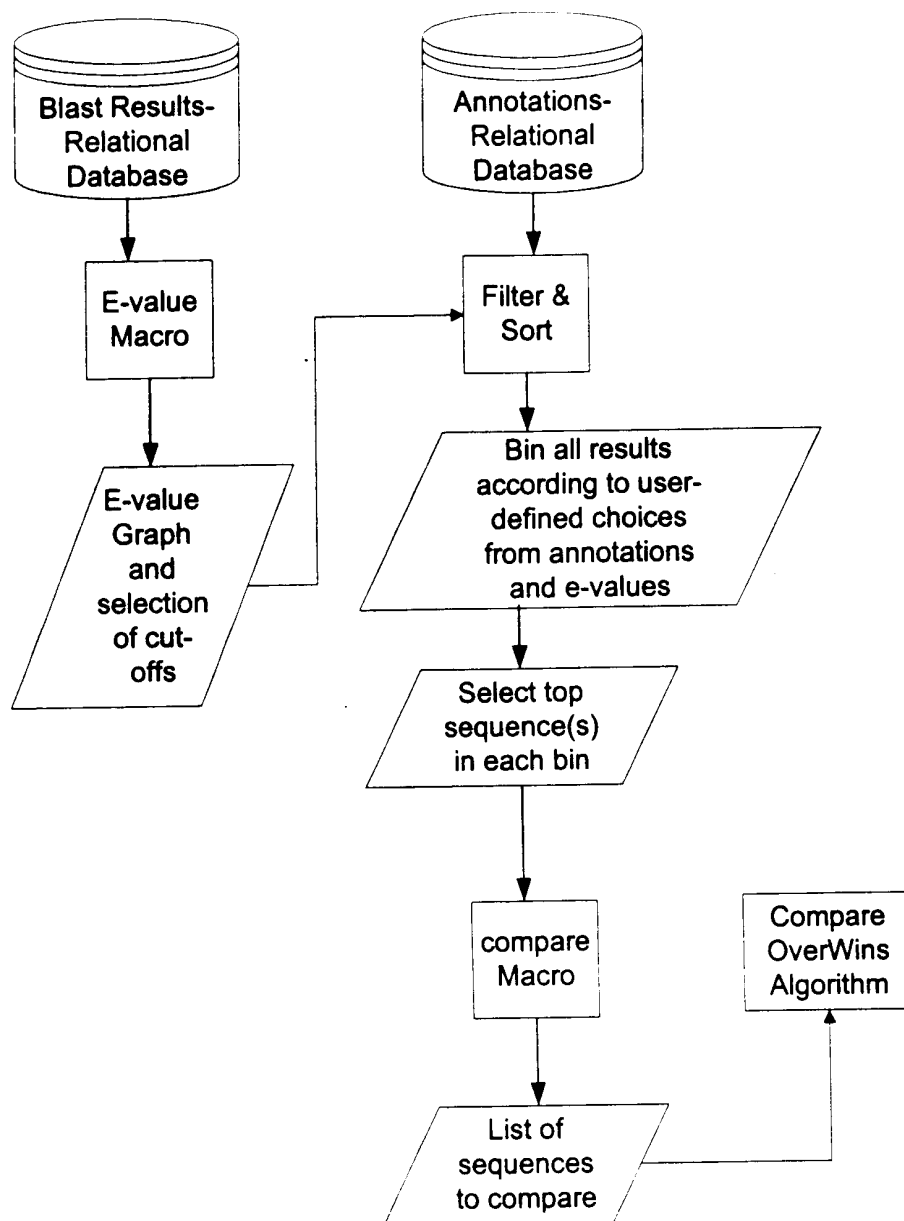


FIGURE 4

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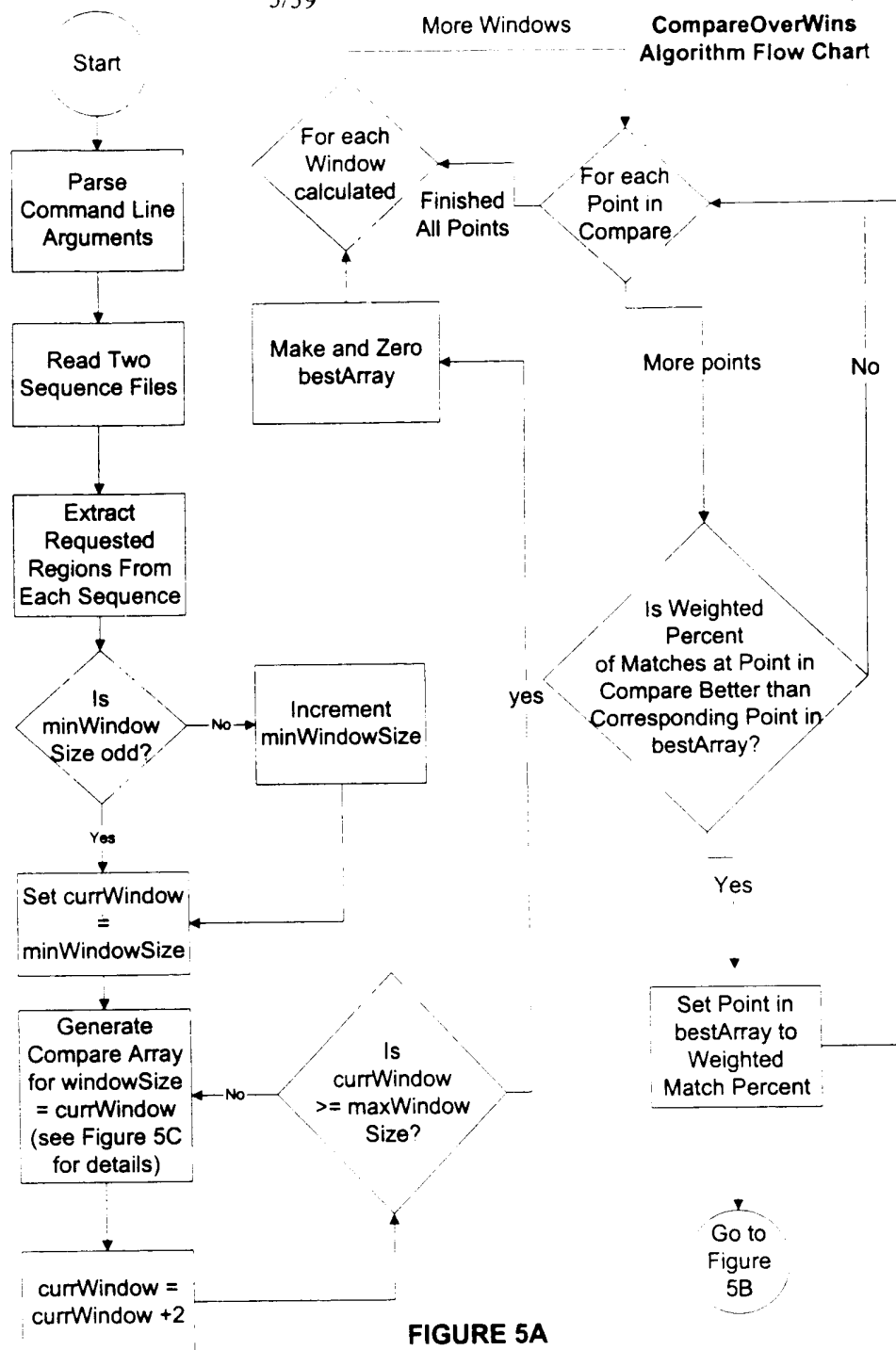


FIGURE 5A

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CompareOverWins
Algorithm Flow Chart

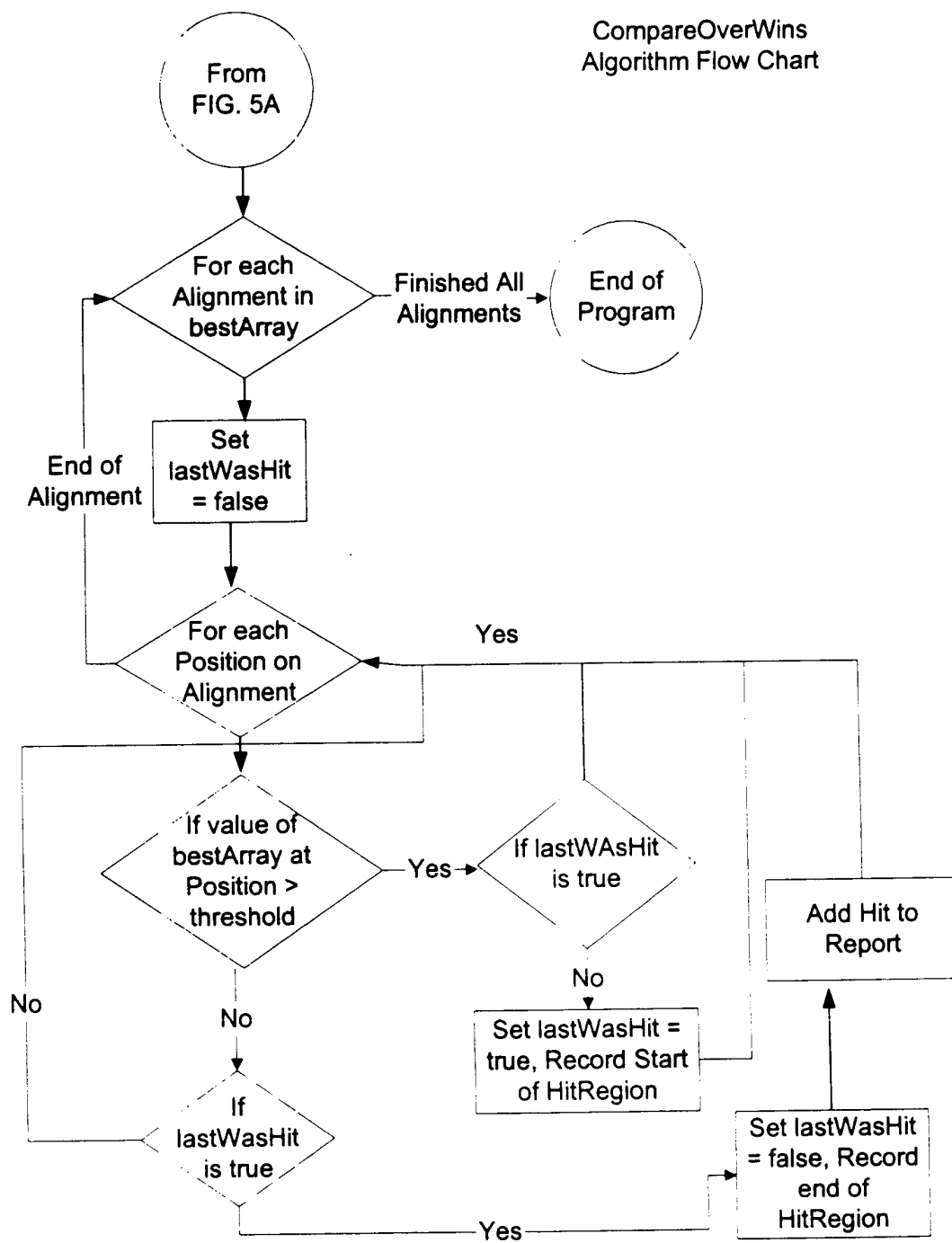


FIGURE 5B

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Input:
 Sequence A length a
 Sequence B length b
 Window Size

CompareOverWins Algorithm Flow Chart Basic Compare

Output:
 Array of size a by b of unsigned chars (0-255)
 Each point represents the number of matches in the
 window at that alignment and position

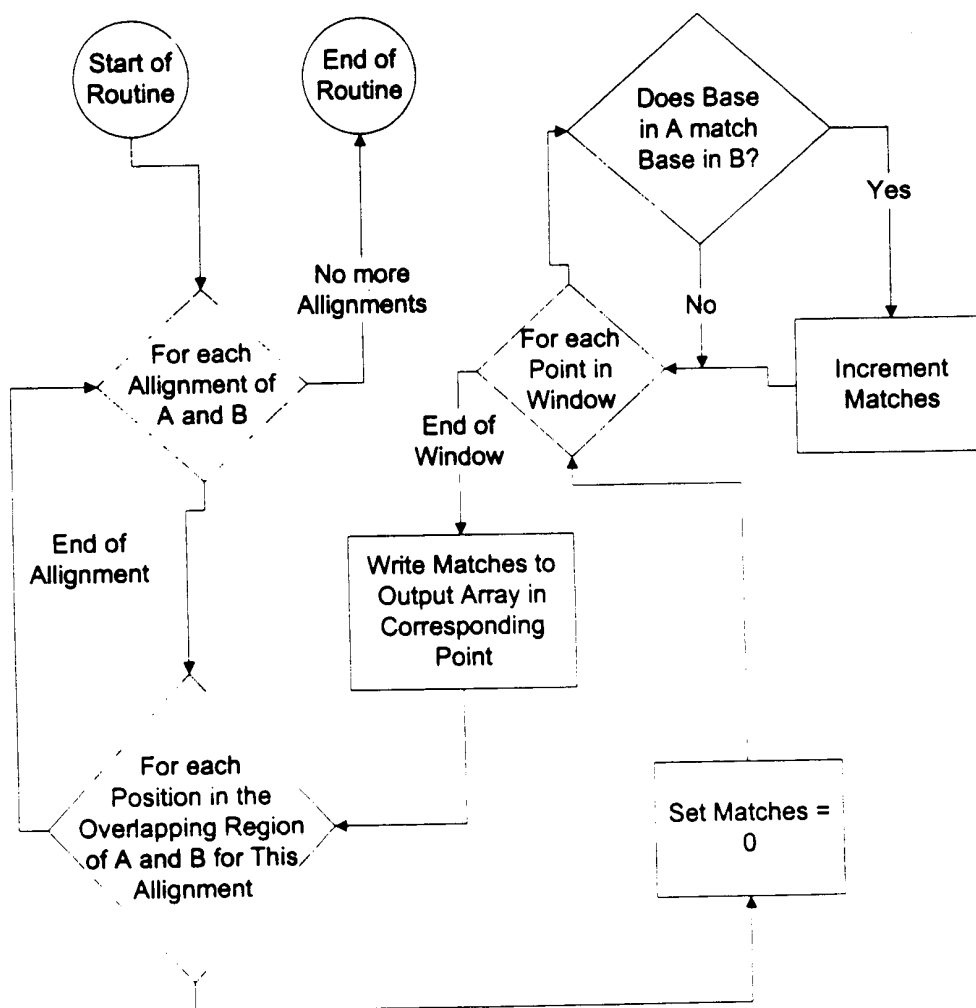
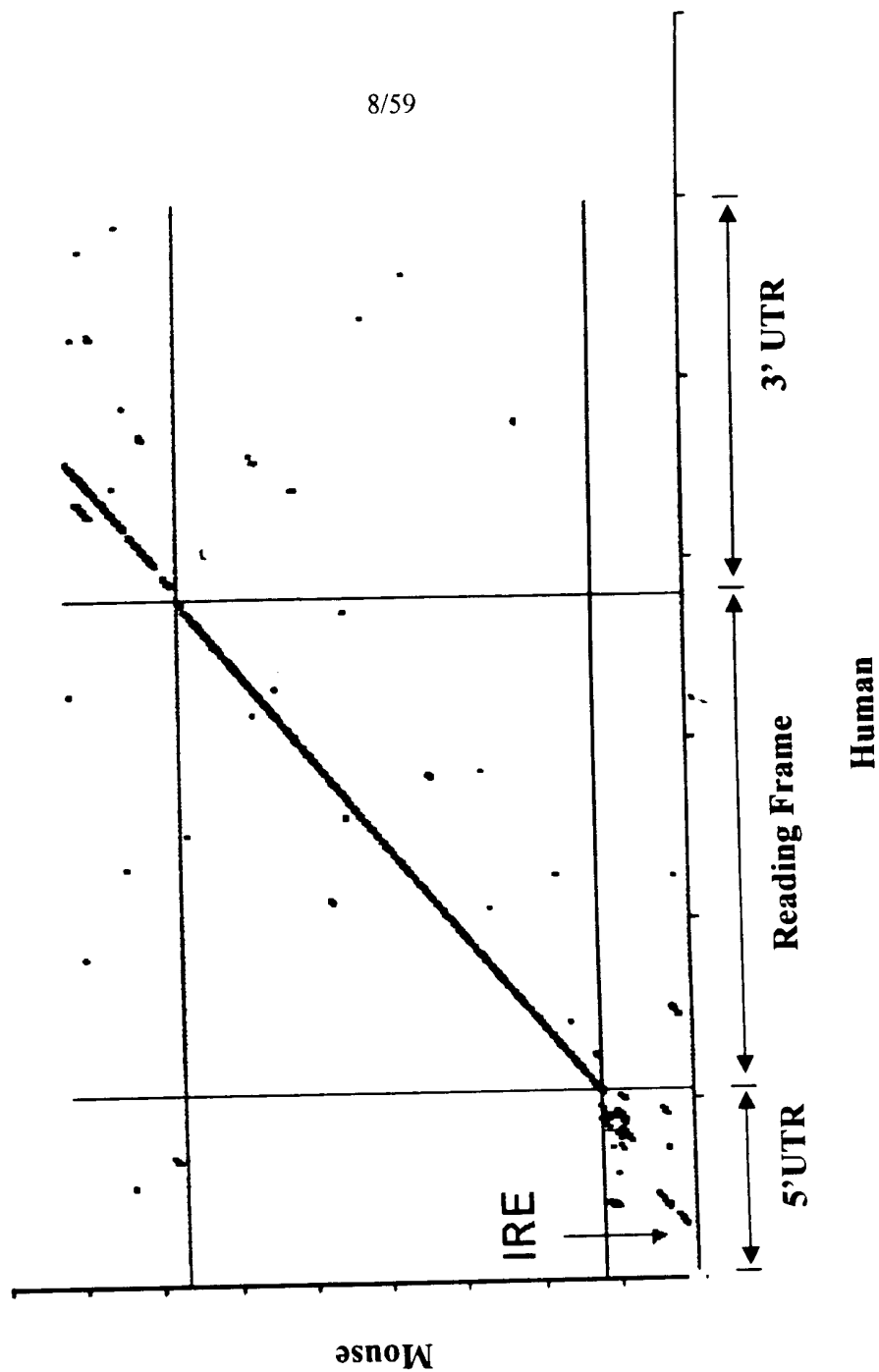


FIGURE 5C

Figure 6



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Self Complementation Analysis - Single Sequence

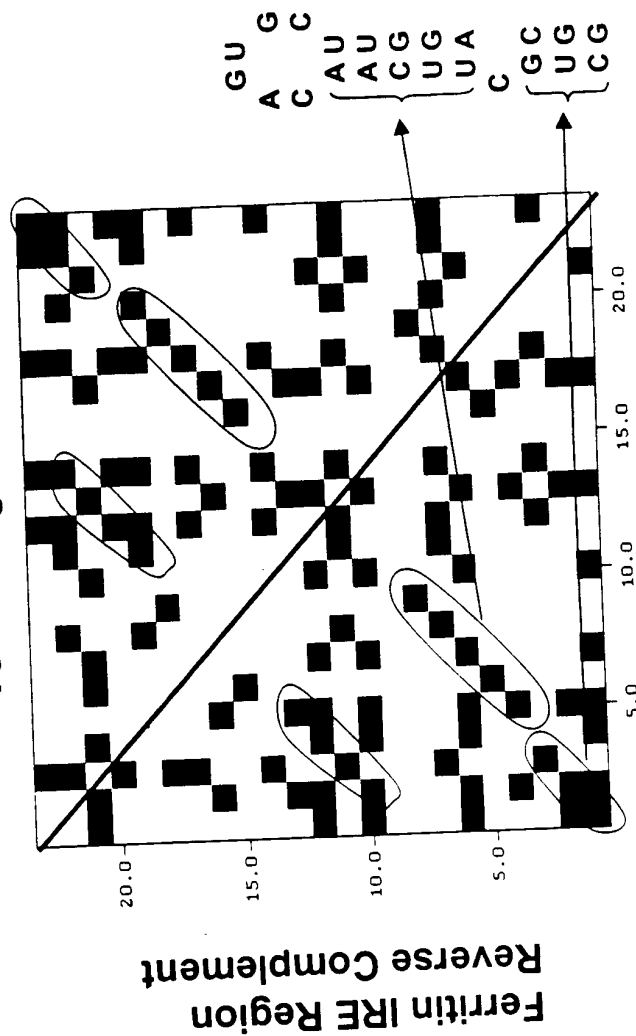
| | | | | | | | | | | | | | | | | | | | | | | | | |
|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|----|
| 3' | G | A | C | G | A | A | G | U | U | G | U | C | A | C | G | A | A | C | C | U | A | C | C | 5' |
| 23 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 22 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 21 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 20 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 19 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 18 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 17 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 16 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 15 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 14 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 13 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 12 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 11 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 10 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 9 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 8 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 7 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 6 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 5 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 4 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 3 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 2 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 1 | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |
| 5' | * | & | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * | * |

Figure 7

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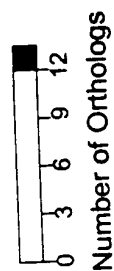
Self Complementarity Comparisons

13 ortholog overlay



Ferritin IRE Region

Figure 8

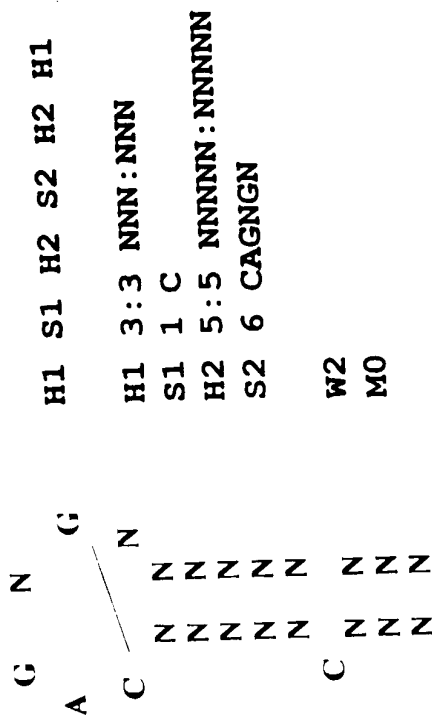


IRE String descriptor

This descriptor allows for

- .. a wobble (W) of 2
- .. no mismatches.
- .. N can be any nucleotide
- .. H refers to the stem region
- .. S refers to the single stranded region.

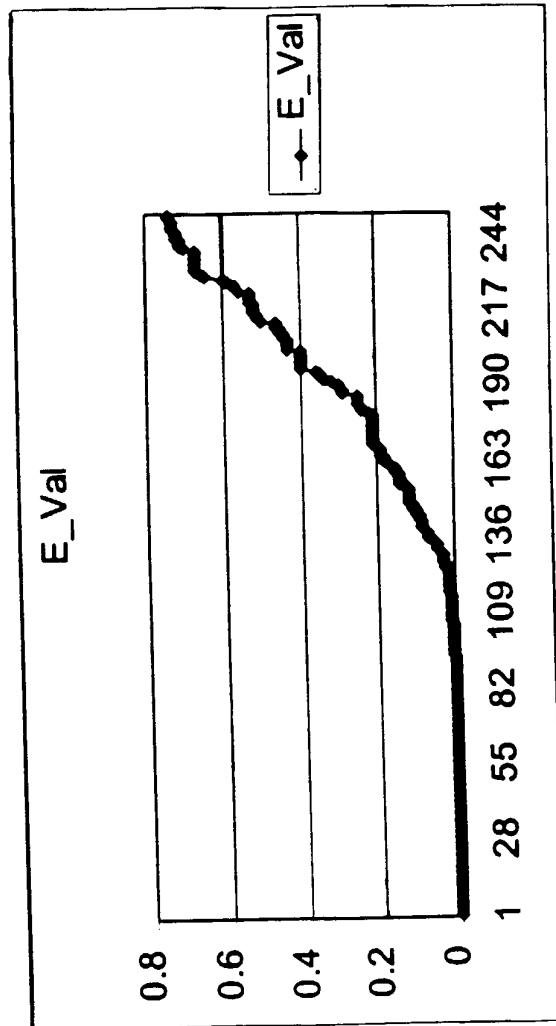
Figure 9



IRE Stem-loop Model

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Figure 10



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Figure 11

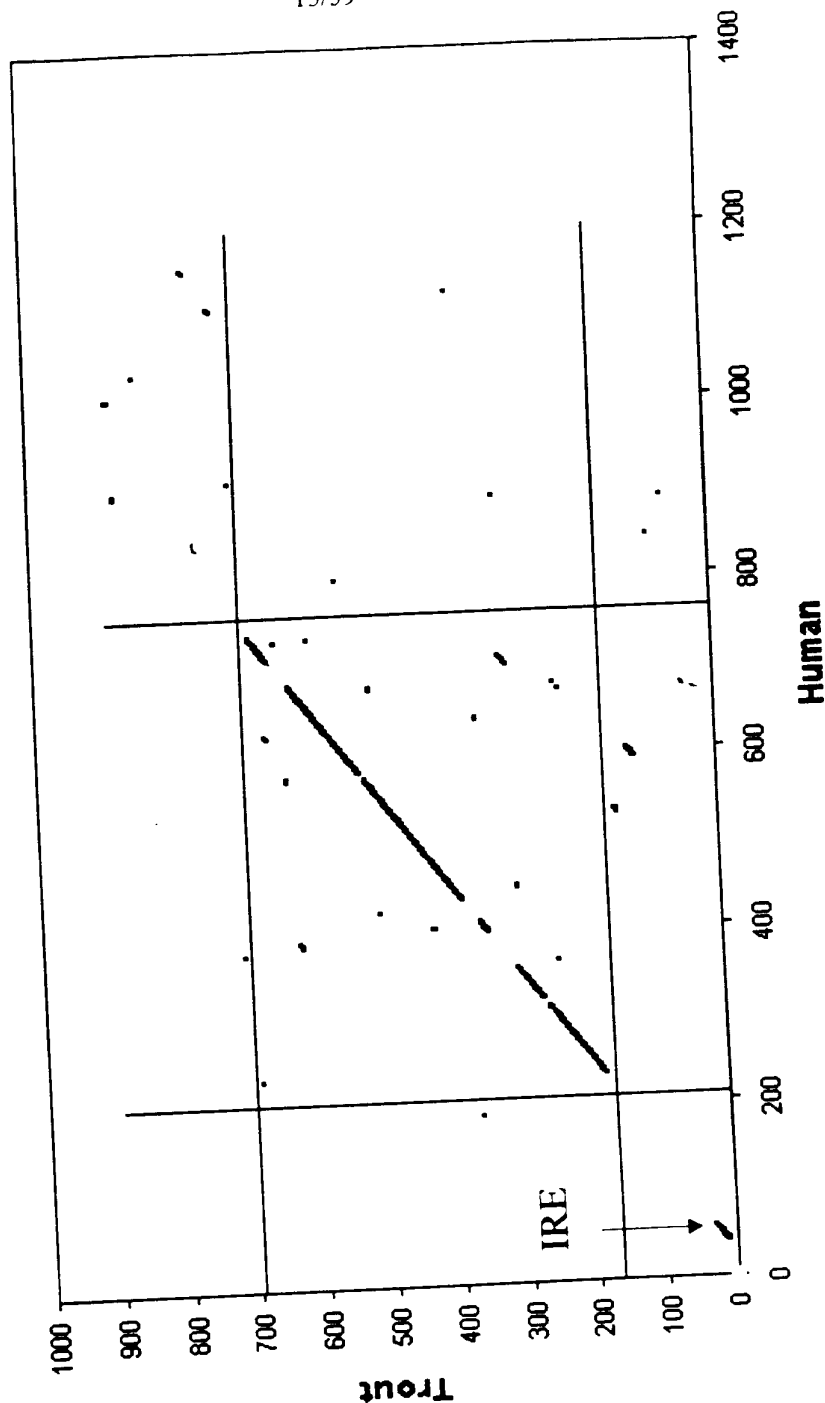
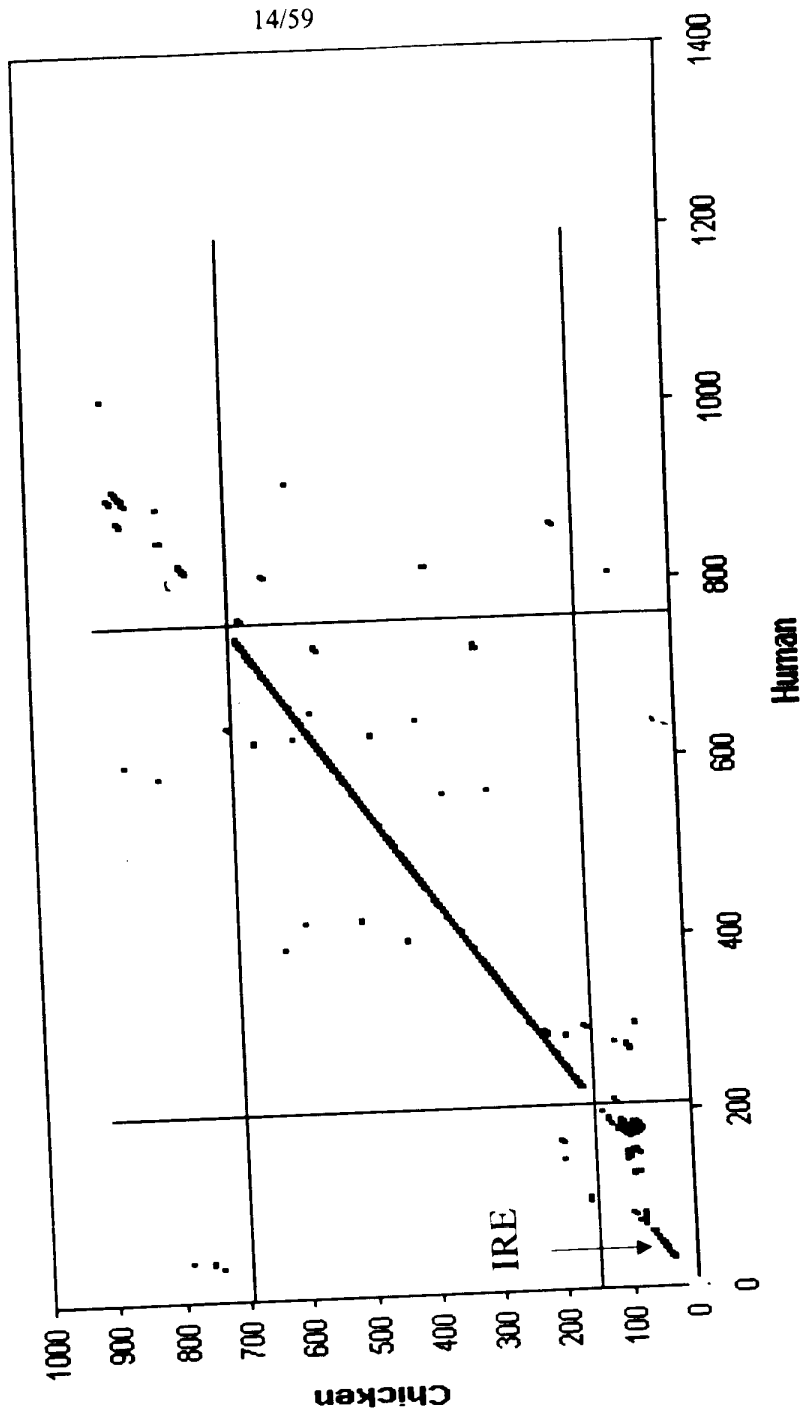


Figure 12



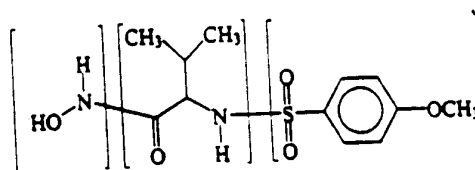
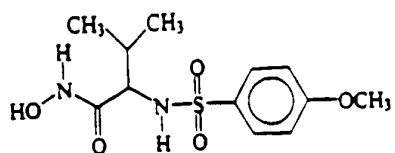
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| | HUMAN PIG | HAMSTER MOUSE RAT | CHICKEN | TROUT SALMON | XENOPUS FROG | FLY | MOSQUITO |
|-------------------------|--------------|-------------------------|-----------|-----------------|-----------------|-----------|-----------|
| HUMAN PIG | GU A C | GU A C | GU A C | GU A C | GU A C | GU A C | GU A C |
| HAMSTER MOUSE RAT | AU AU | AU AU | AU AU | AU AU | AU AU | AU AU | AU AU |
| CHICKEN | CG UG | CG UG | CG UG | CG UG | CG UG | CG UG | CG UG |
| TROUT SALMON | UA UA | UA UA | UA UA | UA UA | UA UA | UA UA | UA UA |
| XENOPUS FROG | C | C | C | C | C | C | C |
| FLY | GC UG | GC UG | GC UG | GC UG | GC UG | GC UG | GC UG |
| MOSQUITO | C | C | C | C | C | C | C |
| | No | No | Yes | Yes | Yes | No | No |
| | | No | Yes | Yes | Yes | No | No |
| | | | No | Yes | Yes | Yes | Yes |
| | | | | No | Yes | Yes | Yes |
| | | | | | No | Yes | Yes |
| | | | | | | No | Yes |
| | | | | | | | No |

Figure 13

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Compound CI



| | | | |
|-------------------|---------|------------|--------------|
| | Fi | Fii | Fiii |
| Molecular formula | H_2NO | C_3H_9NO | $C_7H_7O_3S$ |

Figure 14

Figure 15

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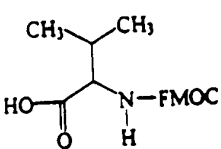
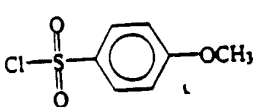
| Reagents | Identifier | Name | Properties |
|---|------------------|-------------------------|------------|
| $\text{H}-\text{O}-\text{NH}_2$ or $\text{P}-\text{O}-\text{NH}_2$ | R _i | Hydroxylamine | ... |
|  | R _{ii} | FMOC blocked amino acid | ... |
|  | R _{iii} | Sulfonylchloride | ... |
| <p>Ⓟ = Solid support</p> | | | |

Figure 16

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Transformation

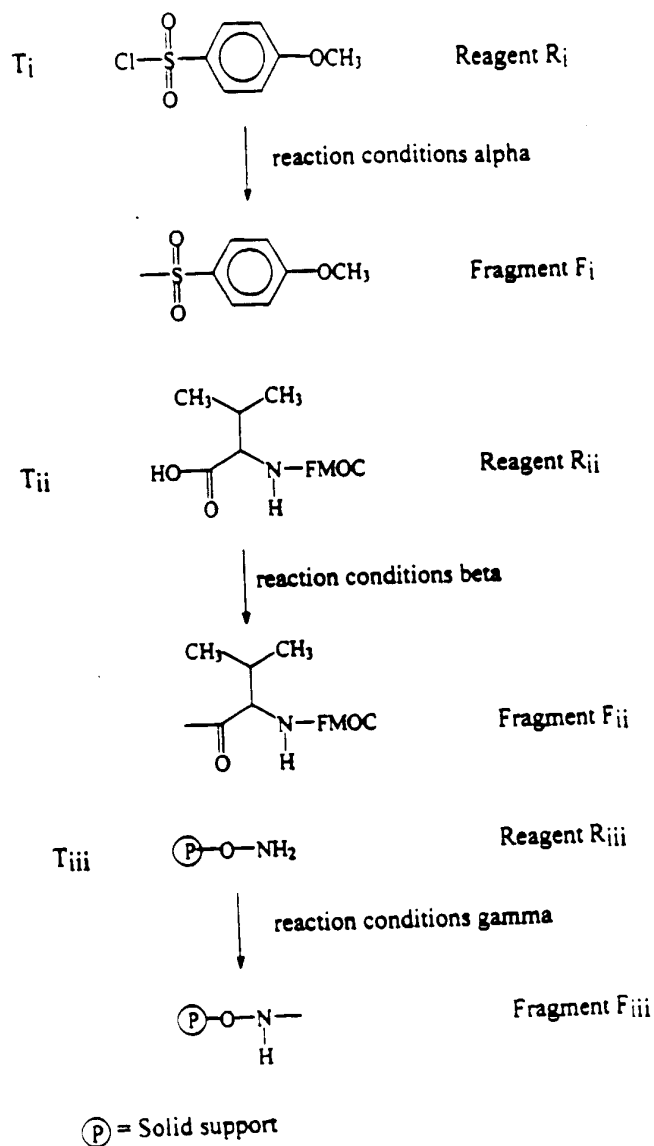


Figure 17

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Common Fragment / Different Reagents and Transformations

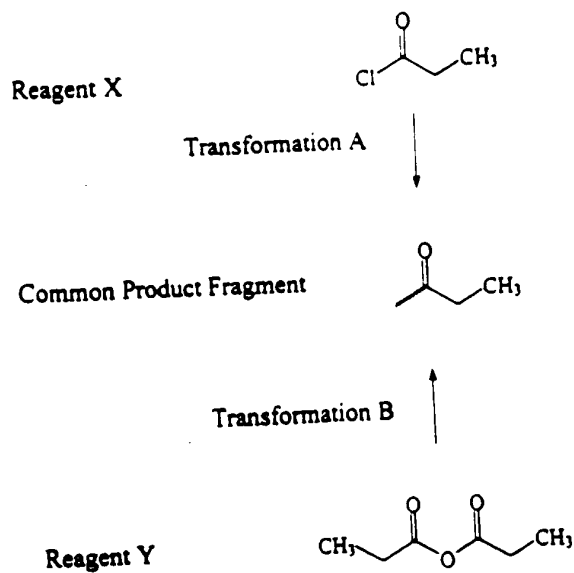


Figure 18

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Common Fragment / Different Reagents and Transformations

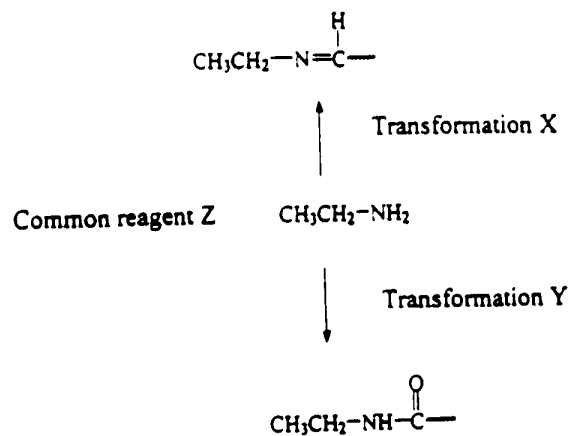


Figure 19A

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Common Reagent

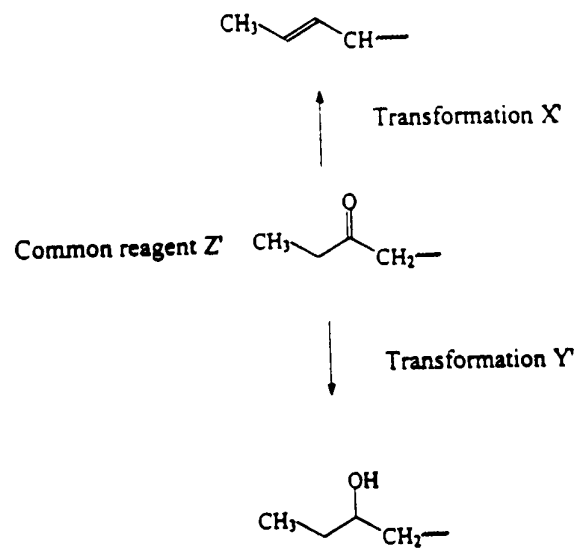


Figure 19B

| <u>Symbolic Structure</u> | <u>Symbolic Identifier</u> | <u>Molecular formula</u> |
|---------------------------|----------------------------|--------------------------|
| | Alcohol | C_2H_5OH |
| | Alkane | C_2H_6 |
| | Alkene | C_2H_4 |
| | Alkyne | C_2H_2 |

Fi'

CuHvNw ...

$$\bigcirc - x$$

Fii'

C_uH_vN_w ...

$$X - \bigcirc - Y$$

Fiii'

CuHvNw ...

CF

C_uH_vN_w ...

Molecular formula F_2

+

Molecular formula F ii'

+

Molecular formula F iii'

= Molecular formula Cl^+

Figure 20

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Symbolic Reagent Table


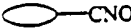


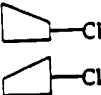
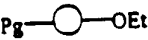
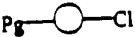

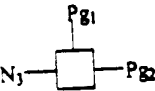
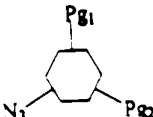
| Identifier | Name | Structure | Molecular formula |
|------------|------|---|-------------------|
| R1 | xxx |  | xxx |
| R2 | ... |  | ... |
| R3 | ... |  | ... |
| R4 | ... |  | ... |
| R5 | ... |  | ... |
| R6 | ... |  | ... |
| R7 | ... |  | ... |
| R8 | ... |  | ... |
| R9 | ... |  | ... |
| R10 | ... |  | ... |

Figure 21

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Symbolic Fragment Table








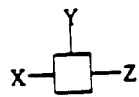
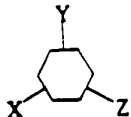
| Identifier | Symbolic Structure | Molecular formula | Molecular Weight |
|------------|--|-------------------|------------------|
| F1 |  | xxx | xxx |
| F2 |  | ... | ... |
| F3 |  | ... | ... |
| F4 |   | ... | ... |
| F5 |  | ... | ... |
| F6 |  | ... | ... |
| F7 |  | ... | ... |
| F8 |  | ... | ... |

Figure 22

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Symbolic Transformation Table










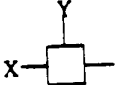
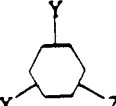
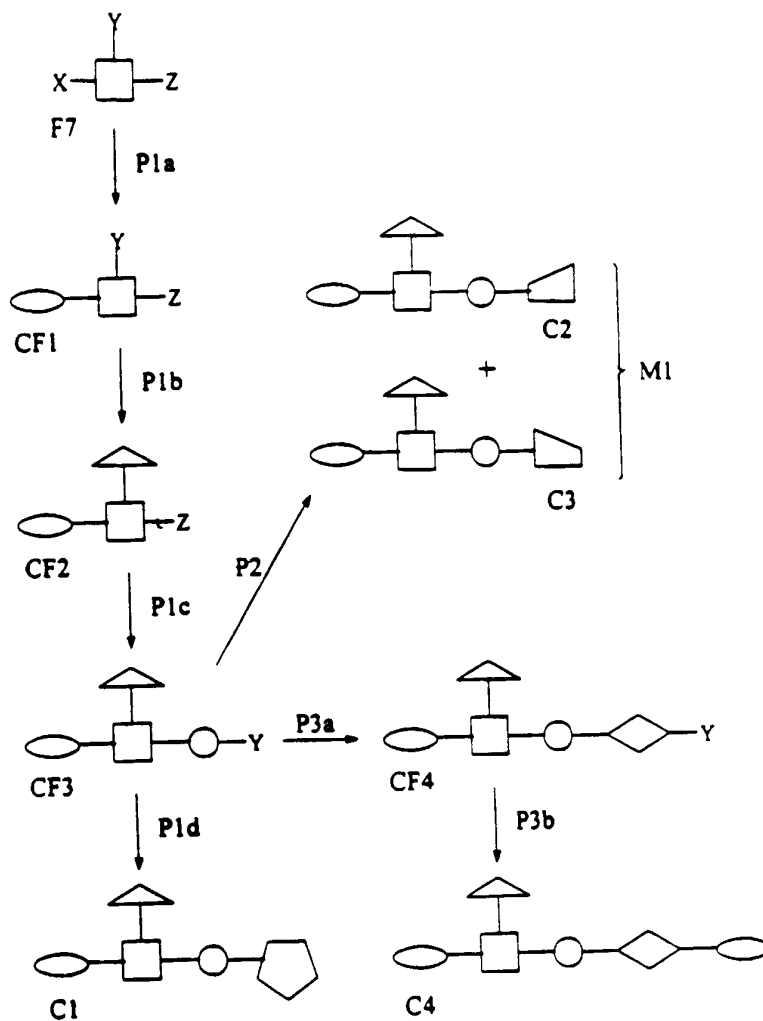
| Identifier | | Symbolic Reactions | Reagent |
|------------|----|---|-----------------------|
| T1 | F1 |  X $\xleftarrow{\quad}$ R1 | conditions α |
| T2 | F2 |  X $\xleftarrow{\quad}$ R2 | conditions β |
| T3 | F3 |  X $\xleftarrow{\quad}$ R3 | conditions α |
| T4 | F3 |  X $\xleftarrow{\quad}$ R4 | conditions α |
| T5 | F4 |  X  X $\xleftarrow{\quad}$ R5 | conditions α |
| T6 | F5 | X —  — Y $\xleftarrow{\quad}$ R6 | conditions ϵ |
| T7 | F5 | X —  — Y $\xleftarrow{\quad}$ R7 | conditions α |
| T8 | F6 | X —  — Y $\xleftarrow{\quad}$ R8 | conditions α |
| T9 | F7 | X —  — Z $\xleftarrow{\quad}$ R9 | conditions γ |
| T10 | F8 | X —  — Z $\xleftarrow{\quad}$ R10 | conditions γ |

Figure 23

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Single Compounds and Mixtures



P = synthetic path CF = complex fragment
 F = fragment M = mixture
 C = compound

Figure 24

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Mixture 2

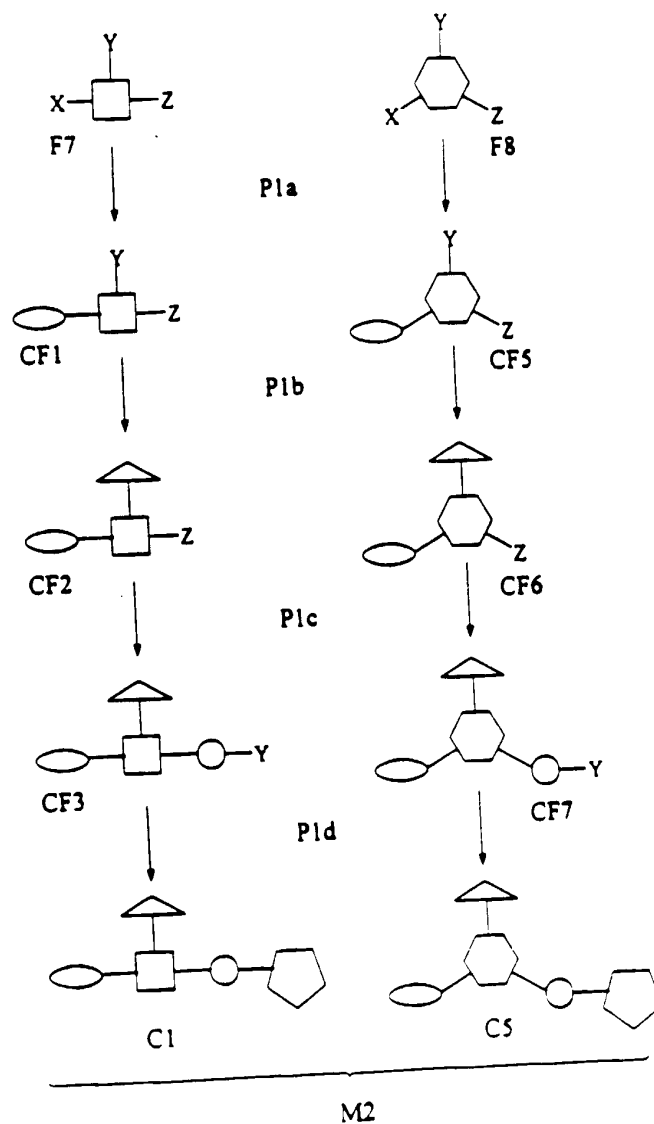


Figure 25

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Mixture 3

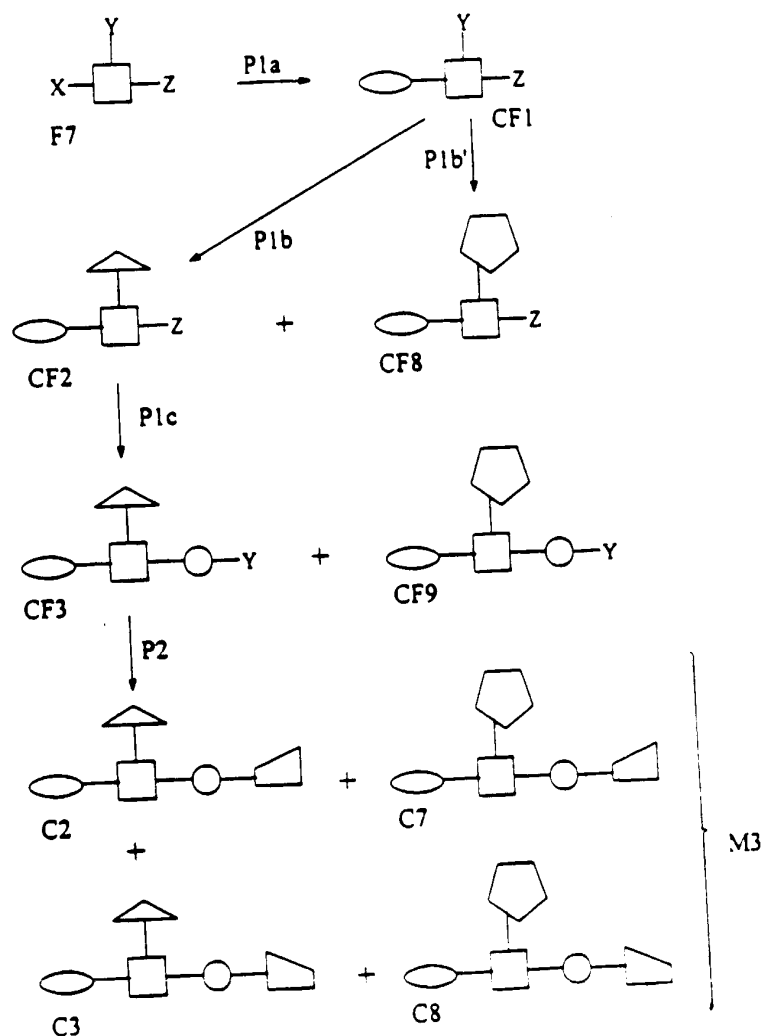
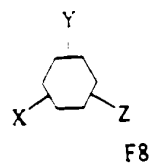
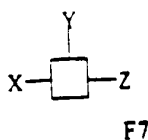


Figure 26

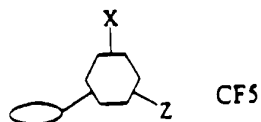
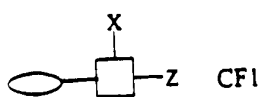
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Mixture 4

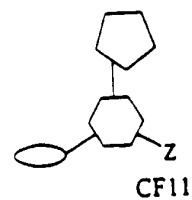
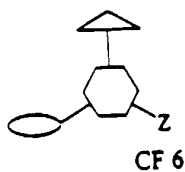
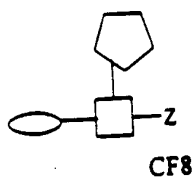
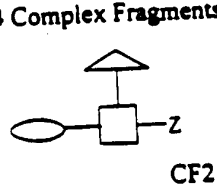
2 Starting Fragments



2 Complex Fragments



4 Complex Fragments



8 Complex Fragments

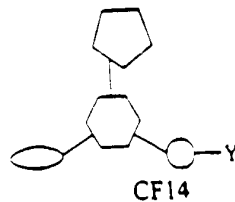
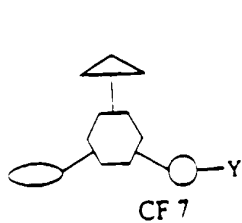
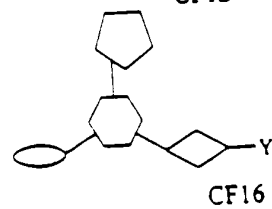
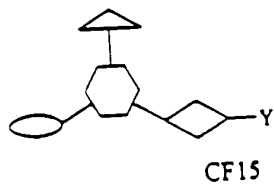
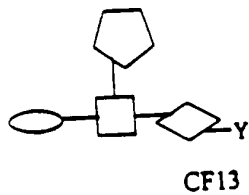
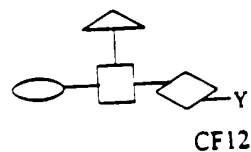
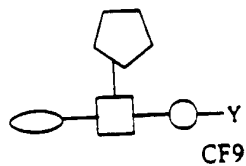
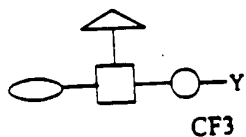


Figure 27A

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Mixture 4 (continued)

16 compounds

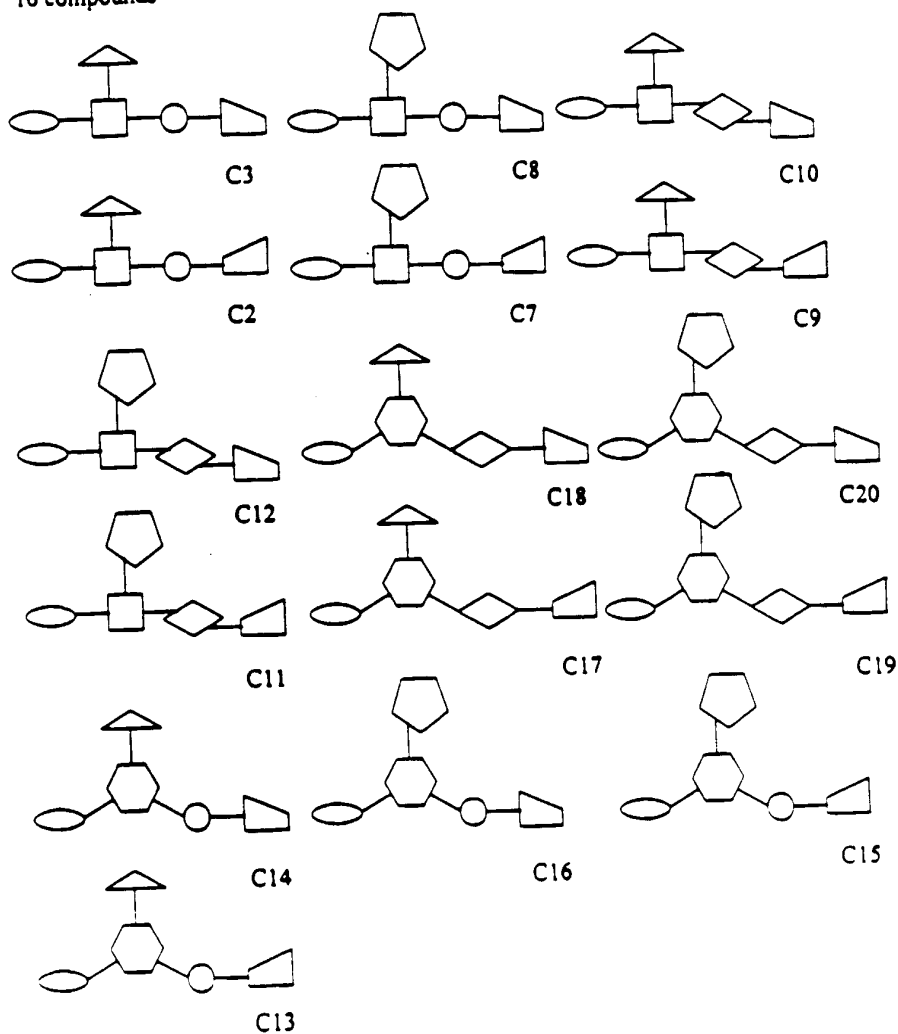


Figure 27B

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Tracking Table for Compound C1

(a) By Fragments:

| n | n+1 | n+2 |
|----|----------------|-----|
| F7 | F2 F1 F5 | F3 |

(b) By Transformations:

Synthesis Path 1

| n | n+1 | n+2 |
|----|----------------|-----|
| T9 | T2 T1 T6 | T3 |

Synthesis Path 2

| n | n+1 | n+2 |
|----|----------------|-----|
| T9 | T2 T1 T7 | T3 |

Synthesis Path 3

| n | n+1 | n+2 |
|----|----------------|-----|
| T9 | T2 T1 T6 | T4 |

Synthesis Path 4

| n | n+1 | n+2 |
|----|----------------|-----|
| T9 | T2 T1 T7 | T4 |

Figure 28

Tracking M1

| Step 1 | | |
|--------|--|--|
| T9 | | |

| Step 2 | | |
|--------|----|--|
| T9 | T2 | |

| Step 3 | | |
|--------|----------|--|
| T9 | T2 T1 | |

| Step 4 | | |
|--------|----------------|--|
| T9 | T2 T1 T7 | |

| Step 5 | | |
|--------|----------------|-----------------|
| T9 | T2 T1 T7 | T5 ¹ |

| Step 5 | | |
|--------|----------------|-----------------|
| T9 | T2 T1 T7 | TS ² |

C3

Figure 29

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Tracking Table

Tracking M2

| Step 1 | | |
|--------|-----|-----|
| n | n+1 | n+2 |
| T9 | | |

| Step 1 | | |
|--------|-----|-----|
| n | n+1 | n+2 |
| T10 | | |

| Step 2 | | |
|--------|-----|-----|
| n | n+1 | n+2 |
| T9 | T2 | |

| Step 2 | | |
|--------|-----|-----|
| n | n+1 | n+2 |
| T10 | T2 | |

| Step 3 | | |
|--------|----------|-----|
| n | n+1 | n+2 |
| T9 | T2 T1 | |

| Step 3 | | |
|--------|----------|-----|
| n | n+1 | n+2 |
| T10 | T2 T1 | |

| Step 4 | | |
|--------|----------------|-----|
| n | n+1 | n+2 |
| T9 | T2 T1 T7 | |

| Step 4 | | |
|--------|----------------|-----|
| n | n+1 | n+2 |
| T10 | T2 T1 T7 | |

| Step 5 | | |
|--------|----------------|-----|
| n | n+1 | n+2 |
| T9 | T2 T1 T7 | T4 |

| Step 5 | | |
|--------|----------------|-----|
| n | n+1 | n+2 |
| T10 | T2 T1 T7 | T4 |

C1

C5

Figure 30

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Tracking Table

Tracking M3

Step 1

| | | |
|----|--|--|
| T9 | | |
|----|--|--|

Step 2

| | | |
|----|----|--|
| T9 | T2 | |
|----|----|--|

Step 3

| | | |
|----|----|----|
| T9 | T2 | T1 |
|----|----|----|

Step 3

| | | |
|----|----|----|
| T9 | T2 | T3 |
|----|----|----|

Step 4

| | | | |
|----|----|----|----|
| T9 | T2 | T1 | T7 |
|----|----|----|----|

Step 4

| | | | |
|----|----|----|----|
| T9 | T2 | T3 | T7 |
|----|----|----|----|

Step 5

| | | | | |
|----|----|----|----|-----------------|
| T9 | T2 | T1 | T7 | T5 ¹ |
|----|----|----|----|-----------------|

C2

Step 5

| | | | | |
|----|----|----|----|-----------------|
| T9 | T2 | T1 | T7 | T5 ² |
|----|----|----|----|-----------------|

C3

Step 5

| | | | | |
|----|----|----|----|-----------------|
| T9 | T2 | T3 | T7 | T5 ¹ |
|----|----|----|----|-----------------|

C7

Step 5

| | | | | |
|----|----|----|----|-----------------|
| T9 | T2 | T3 | T7 | T5 ² |
|----|----|----|----|-----------------|

C8

Figure 31

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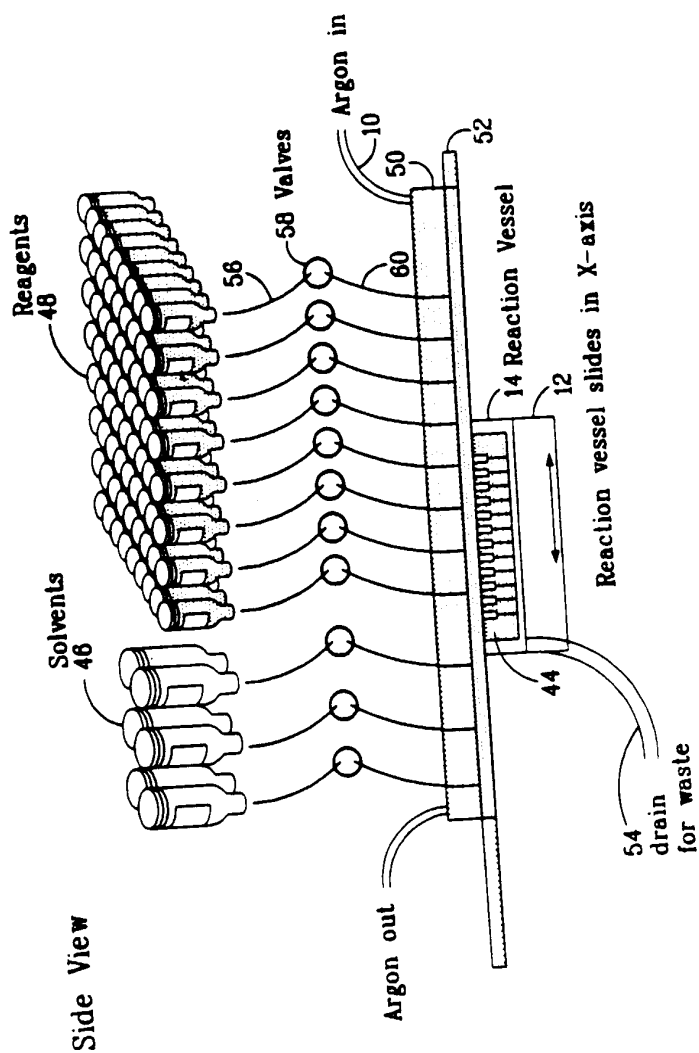


Figure 32

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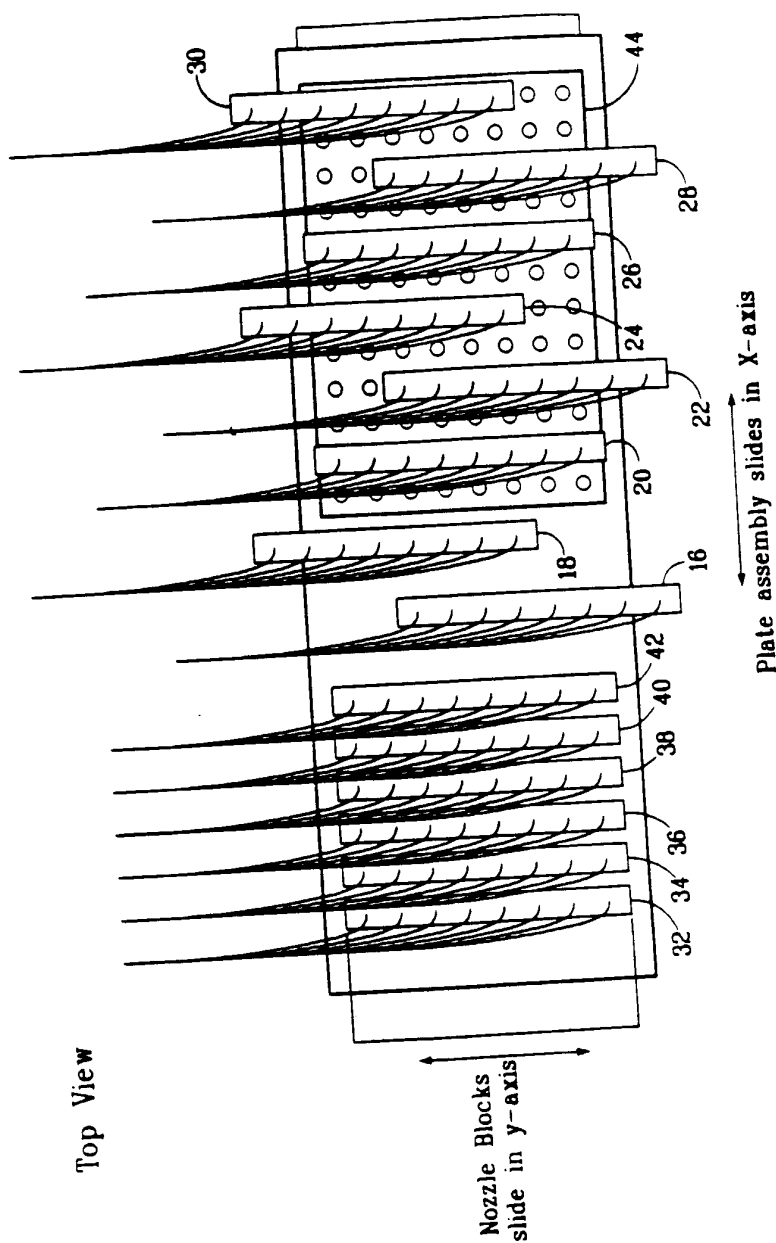


Figure 33

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Synthesis of hydroxamic acids from hydroxylamine resin

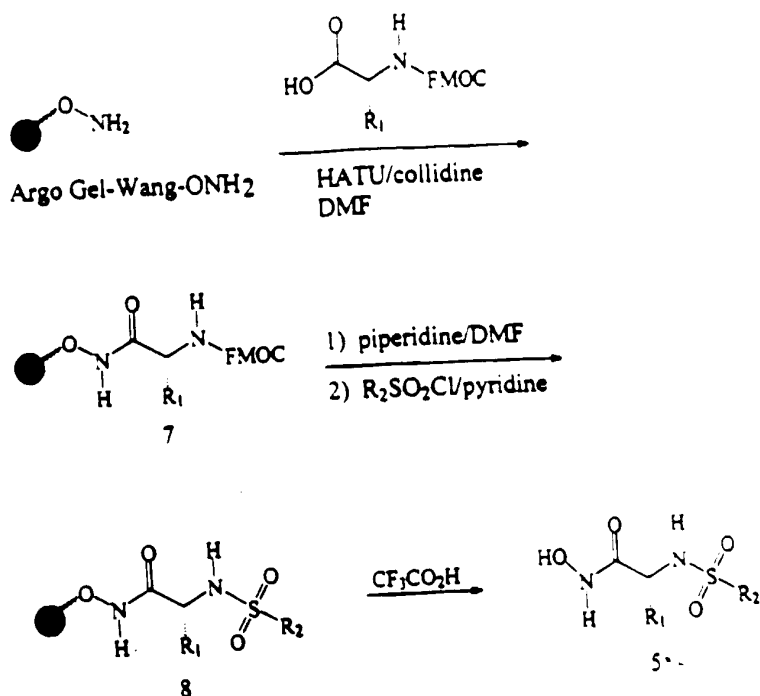
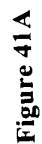


Figure 35



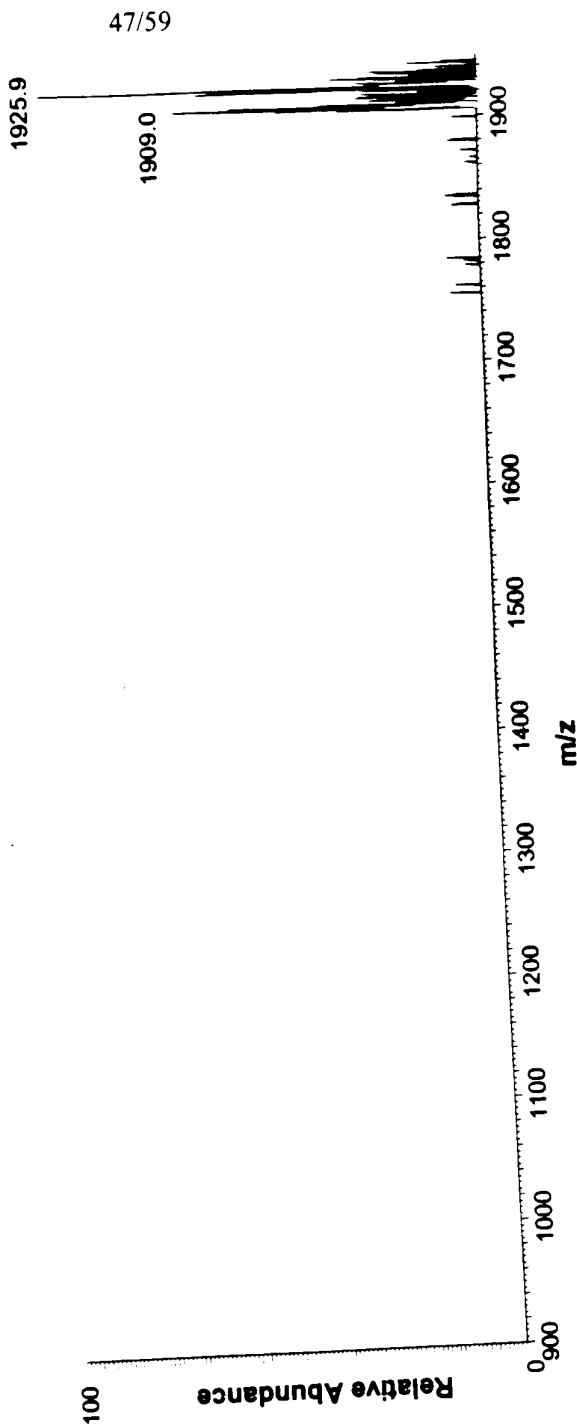


Figure 41B

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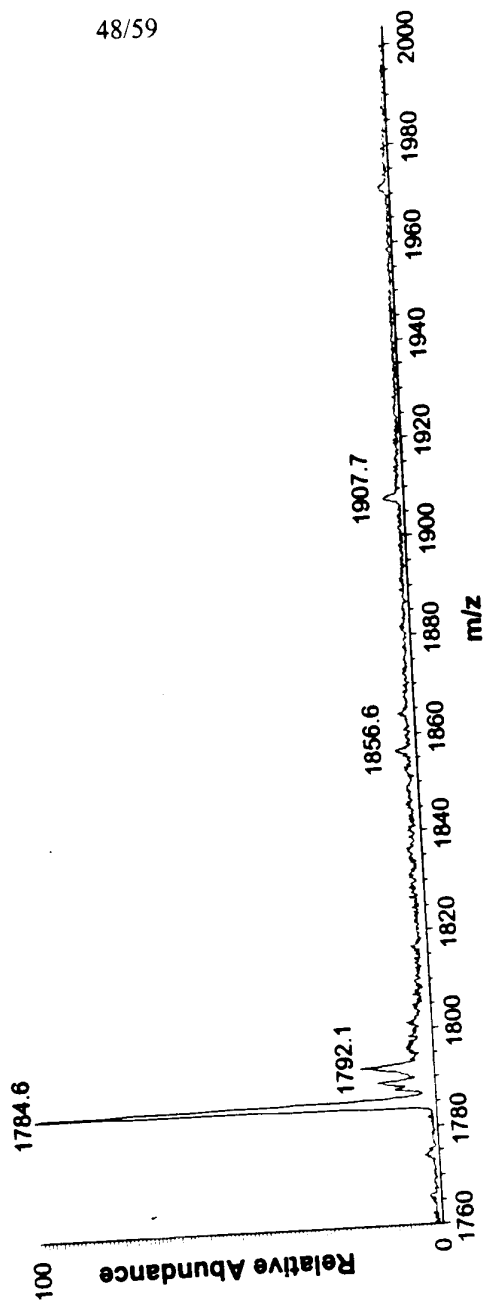


Figure 42A







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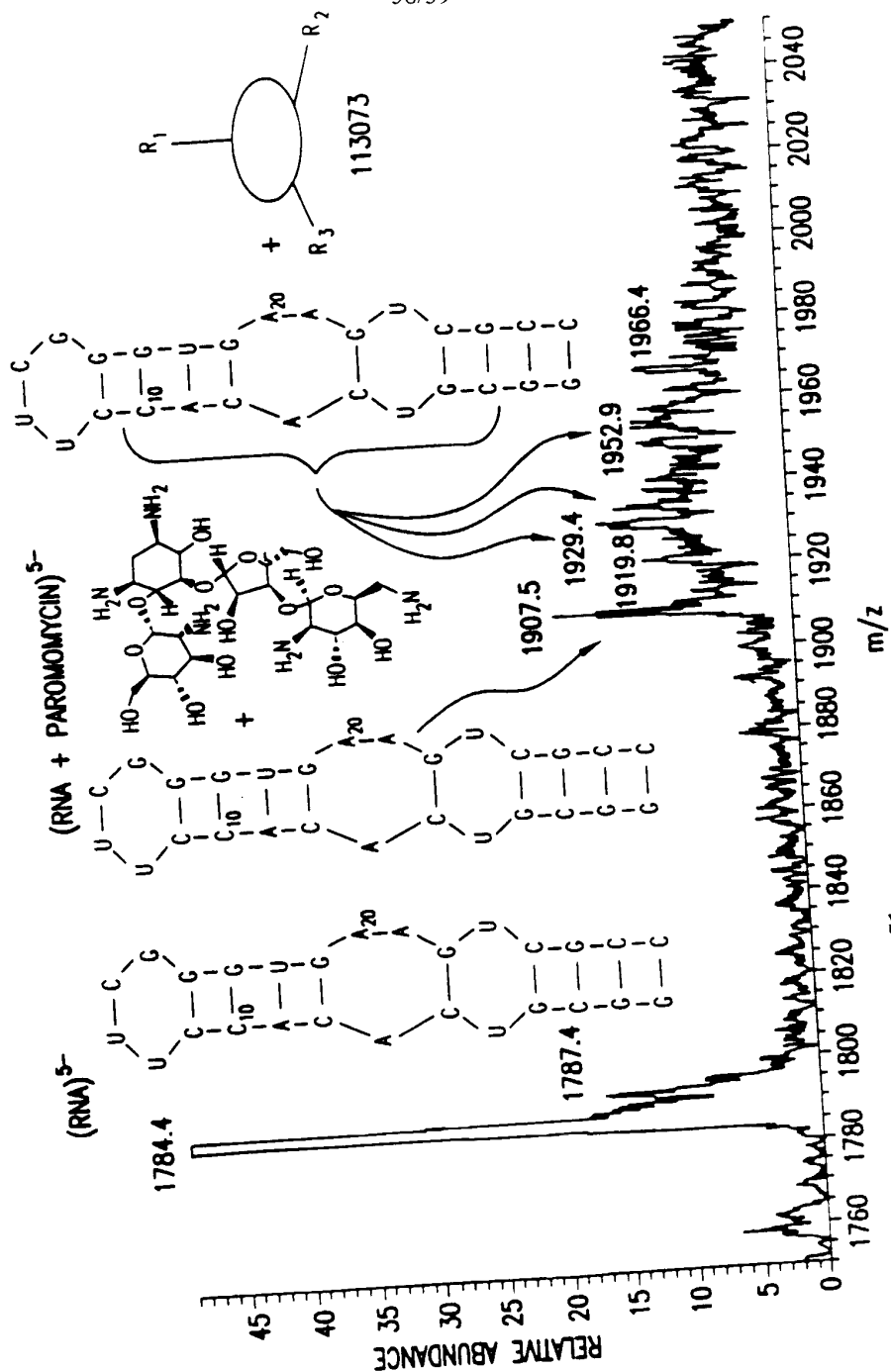


Figure 51

